APPROXIMATION OF THE TEMPERATURE DEPENDENCE OF THE COEFFICIENTS OF INTERDIFFUSION OF VAPOR—GAS SYSTEMS

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The correctness of an approximation equation for the temperature dependence of the coefficients of interdiffusion of vapor—gas systems with a mean deviation of 2% is confirmed by numerous experimental data.

In the modern mathematical theory of inhomogeneous gases the coefficients of interdiffusion D of binary gas mixtures at low pressures are calculated from the equation [1, 2]

$$D = 1{,}883 \cdot 10^{-24} \frac{\sqrt{T^3\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}}{P\,\sigma_{12}^2\,\Omega_D} \tag{1}$$

using the combination rules

$$\sigma_{12} = \frac{1}{2}(\sigma_1 + \sigma_2), \quad \frac{\varepsilon_{12}}{k} = \sqrt{\frac{\varepsilon_1}{k}\,\frac{\varepsilon_2}{k}}\ . \tag{2}$$

But the calculated values of D are obtained with errors exceeding the errors of experimental data even for systems of spherical nonpolar molecules. This can be explained by the fact that the combination rules are insufficiently precise.

The existence of experimental coefficients of interdiffusion in a wide temperature range made it possible to calculate the values of σ_{12} and ε_{12}/k for the Lennard-Jones (6—12) model. The values of σ_{12} and ε_{12}/k were calculated using the method of least squares. The results of the calculation of σ_{12} and ε_{12}/k are presented in Table 1 with an indication of the temperature range of the approximation.

Thus, the values of the coefficients of interdiffusion of vapor—gas systems at 1013 hPa known from the literature and our experimental values were approximated by Eq. (1) with a mean deviation of 2%. The experimental values of the coefficients of interdiffusion are compared with the calculated values in Table 2, where our experimental values of the coefficients of interdiffusion, marked by an asterisk, were obtained by Stefan's method [3] and values of the coefficient of interdiffusion with no literature reference were obtained by the chromatographic method [4].

TABLE 1. Parameters of the Lennard-Jones (6—12) Potential

System	ε_{12}/k, °K	$10^{10}\,\sigma_{12}$, m	Temperature range	System	ε_{12}/k, °K	$10^{10}\,\sigma_{12}$, m	Temperature range
Pentane—CO_2	219,37	4,8218	287÷425	Hexane—Ar	147,34	4,9358	288÷473
Hexane—CO_2	224,42	4,9717	287÷450	Heptane—Ar	137,36	5,1525	290÷443
Heptane—CO_2	175,80	5,4818	290÷425	Octane—Ar	306,78	4,6280	293÷443
Octane—CO_2	556,98	4,3776	302÷425	Iso-octane—Ar	357,86	4,4237	301÷423
Nonane—CO_2	483,09	4,6164	302÷425	Nonane—Ar	245,72	5,0208	301÷423
Decane—CO_2	476,60	4,9605	301÷424	Benzene—Ar	259,52	4,0924	291÷423
Benzene—CO_2	446,71	4,0025	290÷422	Toluene—Ar	325,21	4,1761	292÷423
Toluene—CO_2	360,88	4,3948	302÷443	Acetone—Ar	136,20	4,4158	283÷423
Ethylbenzene—CO_2	319,90	4,8344	301÷425	1-Propanol—He	229,34	3,3132	253÷423
p-Xylene—CO_2	360,07	4,6100	302÷425	1-Butanol—He	446,19	3,1438	313÷523
m-Xylene—CO_2	463,11	4,4254	302÷425	Isobutyl alcohol—He	538,33	3,1042	313÷424
1-Propanol—CO_2	1054,9	3,1936	323÷424	Octane—He	184,52	4,4995	290÷447
1-Pentane—CO_2	521,92	4,0896	290÷443	Toluene—He	160,34	4,0831	293÷523
Pentane—Ar	174,98	4,5695	258÷473				

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TABLE 2. Comparison of Experimental Coefficients of Interdiffusion D with Calculated Values D_c

T, °K	$D \cdot 10^7$, m^2/sec	$\frac{D-D_c}{D} \cdot 100$, %
Pentane–carbon dioxide		
287,0	60,5 [5]	3,2
299,0	65,5*	3,3
302,0	66,12	2,3
311,0	67,6 [5]	—1,2
323,0	74,2 [5]	1,0
344,0	83,2 [5]	0,3
345,0	81,71	—1,6
368,0	94,44	0,6
396,0	106,6	—1,1
425,0	123,4	0,2
Hexane–carbon dioxide		
287,0	51,47*	—2,5
302,0	58,46	0,1
323,2	66,12	—0,5
333,2	70,07	—0,7
345,0	72,16	—3,9
368,0	82,89	—2,2
381,0	90,79	0,3
396,0	99,77	2,4
425,0	111,9	0,6
440,0	120,2	1,2
450,0	125,6	1,4
Decane – carbon dioxide		
301,2	36,00	—3,3
344,6	49,64	0,6
369,9	59,10	3,8
396,2	67,38	2,8
424,0	75,99	1,8
443,2	83,79	1,9
Benzene–carbon dioxide		
290,0	59,9*	0,0
292,9	60,9 [15]	—0,4
298,9	61,0 [6]	—4,5
299,4	63,4 [7]	—0,9
302,0	63,06	—3,3
303,0	65,7 [5]	0,3
303,2	65,70	0,0
314,5	69,1 [7]	—2,4
318,0	72,22	0,0
318,0	71,5 [15]	—1,0
325,0	75,55	0,0
329,3	75,3 [7]	—3,3
345,0	87,60	2,4
368,0	98,68	1,0
381,0	106,2	1,1
396,0	113,0	—0,6
414,0	124,3	—0,3
422,0	128,8	—0,8
1-Propanol–carbon dioxide		
293,2	62,80	—5,3
323,2	80,3 [7]	0,1
343,9	88,72	—0,6
369,9	106,1	1,9
395,9	118,8	0,1
424,2	135,3	—0,5
443,0	146,1	—2,0
Pentane – argon		
258,2	59,7 [10]	—1,1
263,2	61,8 [10]	—1,0
268,2	64,9 [10]	0,0
273,2	67,0 [10]	—0,1
278,2	69,5 [10]	0,0
283,2	72,0 [10]	0,1
288,2	74,3 [10]	—0,1
293,2	77,0 [10]	0,2
298,2	79,2 [10]	—0,2
298,2	89,0 [12]	10,8
Heptane – carbon dioxide		
290,4	47,6*	—0,9
293,2	49,0*	0,2
302,0	50,53	—2,0
345,0	66,06	—0,2
368,6	74,00	—1,0
381,0	80,43	0,9
396,0	88,66	3,4
425,0	95,72	—1,9
Octane–carbon dioxide		
302,0	44,41	—2,0
345,0	59,72	0,3
368,0	69,08	1,5
381,0	72,98	—0,2
396,0	77,10	—2,7
425,0	92,99	1,4
Nonane–carbon dioxide		
302,0	42,41	—2,6
323,0	50,01	0,2
345,0	57,60	0,6
368,0	66,41	1,6
381,0	71,79	2,2
396,0	75,99	0,1
425,0	86,84	—0,8
Toluene–carbon dioxide		
302,0	57,00	—3,0
345,0	77,10	0,6
368,0	87,37	0,1
423,2	115,0	0,1
443,0	123,8	—0,7
Ethylbenzene – carbon dioxide		
301,2	49,31	—2,0
324,4	58,40	0,3
345,0	65,60	—0,2
368,0	76,27	2,1
413,9	94,96	0,9
425,0	99,03	—0,1
p-Xylene–carbon dioxide		
302,0	50,90	—3,5
345,0	69,61	1,0
368,0	78,14	0,0
381,0	84,27	0,9
396,0	90,45	0,7
425,0	101,2	—0,8
m-Xylene–carbon dioxide		
302,0	48,72	—2,0
325,0	57,24	—0,8
368,0	75,38	1,5
381,0	79,48	—0,3
396,0	87,85	1,9
425,0	98,88	—0,5
1-Butanol – carbon dioxide		
302,2	55,11	—5,2
325,0	67,25	0,0
343,9	75,04	—0,8
369,9	88,09	0,4
371,2	87,07	—1,5
381,2	95,90	1,7
395,9	102,1	1,1
418,8	114,1	0,7
424,2	117,0	1,4
443,0	124,0	—1,7

TABLE 2 (continued)

T, °K	$D \cdot 10^7$, m^2/sec	$\frac{D-D_c}{D} \cdot 100$, %
301,0	80,20	—0,8
323,0	95,63	3,3
353,0	109,0	—0,2
353,2	107,5 [8]	—1,5
372,7	115 [12]	—4,3
383,0	124,3	—2,0
403,0	138,7	—0,1
423,0	152,2	0,7
423,2	149 [12]	—1,5
473,2	189 [12]	2,2
Heptane—argon		
290,4	61,4*	0,0
293,5	63,2*	0,9
301,0	65,68	0,1
303,2	65,8 [14]	—1,0
323,0	75,30	0,4
353,0	87,97	—0,1
353,2	84,6 [8]	—3,7
383,0	101,3	—0,3
403,0	111,1	0,2
423,0	120,0	—0,8
443,0	134,0	2,1
Isooctane—argon		
301,0	57,97	0,1
303,2	61,8 [11]	4,6
303,4	59,9 [7]	1,5
323,0	69,44	2,8
353,0	82,16	2,1
382,8	92,38	—1,8
383,0	93,74	—0,4
403,0	104,6	0,7
423,0	112,5	—1,3
Benzene—argon		
288,7	77,4*	0,0
290,9	79,36	1,1
299,7	83 [6]	—0,4
301,0	83,11	—1,0
311,0	89,68	0,0
323,0	95,26	—1,2
353,0	115,6	0,9
373,0	120 [16]	—5,6
383,0	137,1	2,1
403,0	149,0	0,7
423,0	159,1	—1,8
443,0	176,8	0,0
1-Propanol—helium		
253,2	243,2 [7]	—5,5
293,2	337,7 [7]	—1,2
313,2	390,3 [7]	0,4
314,0	400 [9]	2,3
314,2	399,0 [7]	—0,2
323,2	404,6	—2,0
333,2	452,1 [7]	3,2
333,2	432*	—1,3
334,0	449 [9]	2,1
334,2	459,0 [7]	4,0
353,2	473,5	—3,5
353,2	518,1 [7]	5,4
353,6	485,1	—1,2
363,2	540,4 [7]	4,3
392,0	597,0	0,2
423,2	676 [17]	—1,8
423,9	657,1	—5,0
443,2	711 [17]	—5,4
463,2	761 [17]	—6,8
483,2	829 [17]	—5,9
503,2	896 [17]	—5,5
523,2	959 [17]	—6,0
Hexane—argon		
288,6	66,2 [11]	0,2
298,2	84,5 [12]	16,9
301,0	70,76	—0,9
306,5	73,4 [13]	—0,6
323,0	81,63	0,0
353,0	97,09	1,0
353,2	93,4 [8]	—2,5
372,7	107 [12]	1,4
372,9	104,9 [13]	—0,6
383,0	111,4	0,1
403,0	120,9	—0,3
423,0	132,6	0,2
423,2	145 [12]	8,7
473,2	174 [12]	7,3
Octane—argon		
293,2	53,7*	—1,3
301,0	55,37	—3,6
303,0	62,6 [11]	7,1
303,2	58,7 [14]	0,9
323,0	67,13	1,8
333,2	68,98	—1,5
333,6	68,88	—1,9
353,0	81,27	3,4
353,2	72,2 [8]	—8,9
383,0	89,94	—2,4
403,0	101,6	0,0
423,0	112,6	0,8
443,0	120,1	—1,7
Nonane—argon		
301,0	51,33	—3,8
323,0	62,01	1,3
353,0	74,15	1,9
383,0	84,01	—1,1
403,0	93,96	0,5
423,0	102,1	—0,2
Toluene—argon		
292,0	64,6*	—2,3
301,0	70,69	0,5
323,0	82,30	1,5
353,0	99,87	3,0
383,0	110,8	—2,8
393,0	119,0 [16]	—0,7
403,0	126,3	0,3
423,0	139,2	0,6
Acetone—argon		
283,2	87,5*	—0,5
299,5	98 [6]	—0,1
300,0	98,00	—0,2
301,0	99,18	0,4
323,0	112,7	0,2
363,0	139 [16]	0,2
383,0	152,0	0,0
403,0	168,7	1,4
423,0	184,7	1,8
1-Butanol—helium		
313,2	287,9 [7]	—7,7
323,2	319,0	—3,7
333,2	338,7 [7]	—4,1
353,2	393,4	—1,0
373,2	440,1 [7]	—1,1
392,0	503,0	2,3
423,2	587 [17]	2,3
423,9	591,0	2,7
443,2	653 [17]	3,9
463,2	689 [17]	0,8
483,2	746 [17]	0,7
503,2	792 [17]	—0,8
523,2	841 [17]	—1,8

TABLE 2 (continued)

T, °K	$D \cdot 10^7$, m^2/sec	$\frac{D-D_c}{D} \cdot 100$, %	T, °K	$D \cdot 10^7$, m^2/sec	$\frac{D-D_c}{D} \cdot 100$, %
Octane–helium			Isobutyl alcohol–helium		
290,4	193*	—1,8	313,2	277,5 [7]	—3,7
323,2	240,1 [4]	0,1	334,0	331,0 [9]	1,0
353,2	296,9 [4]	4,4	333,2	320,1 [7]	—2,3
373,2	320,3	1,9	353,2	355,1 [7]	—3,3
392,0	336,5 [4]	—2,0	354,0	355 [9]	—4,1
423,2	391,4 [4]	—1,1	373,2	416,6 [7]	1,5
435,0	412,2	—1,0	424,0	553,3	3,8
447,0	432,4	—1,0	Toluene–helium		
			293,2	250,3	—2,6
			323,2	303,1 [4]	—1,8
			353,2	369,0 [4]	1,3
			370,3	395,7	—0,5
			373,6	411,5 [4]	1,8
			391,9	444,1	0,7
			423,2	501,3 [4]	—0,9

The experimental data obtained by Stefan's method are the result of fivefold measurements; the data of the chromatographic method are arithmetic-mean values of 7-10 measurements.

Some coefficients of interdiffusion contained in [12] differ (up to 16.9%, see Table 2) from the results of other authors and from our data. This is explained by the fact that high carrier-gas velocities were used in [12], for which overstated values are obtained.

NOTATION

D, coefficient of interdiffusion, m^2/sec; T, temperature, °K; M_1 and M_2, molecular masses of components 1 and 2; P, absolute pressure, hPa; σ_{12} and ε_{12}/k, parameters of the interaction potential of different molecules, m and °K; k, Boltzmann constant, J/°K; $\Omega_D = f(kT/\varepsilon_{12})$, reduced collision integral of the Lennard-Jones (6—12) potential under consideration; σ_1, σ_2 and ε_1/k, ε_2/k, parameters of the interaction potential of identical molecules, m and °K.

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GASDYNAMIC FUNCTION CHARACTERIZING THE FLUX MOMENTUM EXPRESSED IN TERMS OF VARIOUS PARAMETERS APPROPRIATE TO DISSOCIATING NITROGEN TETROXIDE

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Various expressions for an important gasdynamic function characterizing the gas-flux momentum are obtained.

The present investigation, in which various expressions for the flux momentum are derived, is a continuation of [1], where a series of gasdynamic functions was considered.

The function expressing the momentum of a flux is written in the form

$$J = G\omega + pF. \tag{1}$$

But since G = ρwF, it follows that

$$J = G\left(\omega + \frac{p}{\rho\omega}\right). \tag{2}$$

In [1], the following expressions were obtained:

$$a_{cr}^2 = \xi_{cr}^2 2\,\frac{k}{k+1}\,\frac{R}{\mu_{N_2O_4}}\,T_0 \tag{3}$$

and

$$\frac{T_0}{T} = \left\{1 + \frac{1}{\eta}\,\frac{k_T - 1}{k_T}\,[(Z_{ef})_{p,T} - (Z_{ef})_{p_0,T}]\right\}\left(1 - \frac{1}{\eta}\,\frac{k_T - 1}{k_T}\,\frac{k}{k+1}\,\xi_{cr}^2\lambda^2\right)^{-1}, \tag{4}$$

where

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